Bound states in the phase diagram of the extended Hubbard model

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The paper shows how the known, exact results for the two electron bound states can modify the ground state phase diagram of extended Hubbard model (EHM) for on-site attraction, intersite repulsion and arbitrary electron density. The main result is suppression of the superconducting state in favor of normal phase for small charge densities.

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I. INTRODUCTION

The Hubbard model appears in almost all areas of solid state physics. Its universality is connected with the fact that it describes both band movement of charges as well as local and nonlocal – in the extended model – correlations [1]. Treating its parameters as effective ones, the model has been used in research of magnetism, superconductivity and especially high temperature superconductivity (HTS), other various phenomena in the solid, charge orderings, phase separation etc., in materials like high temperature superconductors, bismuthates, Chevrel phases, amorphous semiconductors, heavy fermion materials, systems with alternating valence to name the few (for a review see, e.g., Ref. [2]).

Unfortunately there are not many exact results concerning this model. Usually the results are obtained in specific limits: infinite dimensions, one dimension (the most numerous group), infinite repulsion, half-filled band or other specific band fillings. We can mention the exact solution in one dimension ($d = 1$) obtained by Bethe ansatz [3], Lieb's ferrimagnetism [4], Nagaoka ferromagnetism in repulsive, half-filled systems with one hole [5], flat band ferromagnetism [6], some bounds on correlation functions [7, 8, 9] and a finding of Randeria [10], according to which, existence of two-electron bound states of s-wave symmetry is necessary and sufficient condition for appearance of s-wave superconductivity in $d = 2$ systems with low electron density. Let's also note that the mean-field BCS equations for superconductivity in the Hubbard model with effective attractive interaction between electrons, in the limit of vanishing electron density turn into Schrodinger equations, which can also be solved exactly [11].

A phase diagram in two dimensions for arbitrary n, a case of special interest due to the possible connection with high temperature superconductivity, is still under examination. The results obtained in the mean-field approximation show competition of phases: in half-filled band charge density waves (CDW) for $W \geq 0$, superconductivity for $U < 0$ and spin density waves for $U > 0$ [2]. The calculations for $n \neq 1$ suggest possibility of phase separation for $U < 0$ [2, 12]: electron droplets for large enough $W < 0$ and phase separation of CDW (with $n = 1$) with SS for $W > 0$ (PS[CDW/SS]), for n around half-filled band competing with the pure SS state in low density limit.

This paper shows, how the known solutions for the bound states (including exact solutions of Schrodinger equation) can be used for modification of the ground state phase diagram of the extended Hubbard model.

II. HAMILTONIAN AND THE SUPERCONDUCTING STATE

We begin with the extended Hubbard Hamiltonian in standard notation:

$$H = \sum_{ij\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \frac{1}{2} W \sum_{ij} n_{i\sigma} n_{j\sigma'} - \mu \sum_{i} n_i \ , \tag{1}$$

where we sum over nearest-neighbors (nn) sites only. U and W are treated as effective parameters. We use broken-symmetry Hartree-Fock approach (for details see Ref. [13]). As we are interested in the properties of the superconducting state, we introduce averages of operators $c_{-k\downarrow} c_{k\uparrow}$ in Wick's-type decoupling [14] of the four-operator terms in the Hamiltonian. Non-zero average of such pair-creating operators means phase-coherence among pairs, i.e. a presence of superconducting state, and serves as an order parameter (see Eq. (3)).

$$H_0 = \sum_{k\sigma} (\varepsilon_k - \overline{\mu}) c^{\dagger}_{k\sigma} c_{k\sigma} + \sum_{k} (\Delta_k c^{\dagger}_{k\uparrow} c^{\dagger}_{-k\downarrow} + h.c.) + C \ , \tag{2}$$

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where:

$$\Delta_{k_1} = \frac{1}{N}\sum_{k_2}(W_{k_2-k_1}+U)\langle c_{-k_2\downarrow}c_{k_2\uparrow}\rangle \ , \tag{3}$$

and $\overline{\mu} = \mu - (\frac{U}{2} + zW)n$, where z is coordination number of hypercubic lattice, $W_k = W\gamma_k$, $\varepsilon_k = -t\gamma_k$, $\gamma_k = 2\sum_\alpha^d \cos k_\alpha$, $\alpha \in (x, y, z)$. After diagonalization of the Hamiltonian Eq. (2) we obtain quasiparticle energy:

$$E_q = \sqrt{(\varepsilon_q - \overline{\mu}\ )^2 + |\Delta_q|^2}\ . \tag{4}$$

and a self-consistent equation for the gap:

$$\Delta_k = \frac{1}{N}\sum_q (W_{k-q}+U)\frac{\Delta_q}{2E_q}\tanh\frac{\beta E_q}{2}\ , \tag{5}$$

where $\beta = 1/k_BT$, T is temperature and k_B Boltzmann constant. The constant C in the Hamiltonian Eq. (2) can be expressed now as:

$$C = -\frac{1}{4}(U+2Wz)n^2 + \frac{1}{N}\sum_k \frac{|\Delta_k|^2}{2E_k}\tanh\frac{\beta E_k}{2}\ , \tag{6}$$

The pairing potential in the singlet channel (see Eq. (3)) takes on the separable form for the square lattice and nn interaction: $U + W_{k_1-k_2} = U + W\gamma_{k_1}\gamma_{k_2}/z$ (retaining only the terms of s-wave symmetry), and that makes possible solving Eq. (3) by an ansatz:

$$\Delta_k = \Delta_0 + \Delta_\gamma\gamma_k\ , \tag{7}$$

what leads us to the set of self-consistent equations:

$$\Delta_0 = -U\frac{1}{N}\sum_q(\Delta_0 + \gamma_q\Delta_\gamma)F_q\ , \tag{8}$$

$$\Delta_\gamma = -\frac{W}{z}\frac{1}{N}\sum_q \gamma_q(\Delta_0 + \gamma_q\Delta_\gamma)F_q\ , \tag{9}$$

$$n - 1 = -\frac{2}{N}\sum_q(\varepsilon_q - \overline{\mu})F_q\ . \tag{10}$$

where $F_q = (\tanh\frac{\beta E_q}{2})/2E_q$. In the case of the rectangular density of states (DOS) and pure on-site pairing we can obtain analytical solutions [12]; in the case of the extended s-wave superconductivity (Eqs (8) – (10)) analytical solutions exist in the limit of low electron density. Introducing a new parameter: Δ_γ/Δ_0, we can expand Eqs (8) – (10), treating Δ_0 as a small parameter. As a result we obtain a formula for critical value for appearance of superconductivity for given U and n in the ground state [15]:

$$W_{cr} = \frac{8t^2}{\mu(1-n) + 8tI - 2\mu^2/U}\ , \qquad \text{where} \qquad I = \int_{-1}^{\mu/D} x\rho(x)\ dx\ , \tag{11}$$

and $D = zt$ is half-bandwidth unit. In the case of rectangular DOS this formula reduces to [16]:

$$W_{cr}(1 + (n-1)^2(1 + 16t/U)) = -4t\ . \tag{12}$$

We can go a step further in our mean-field analysis and include Fock term $p = \frac{1}{N}\sum_{k\sigma}\gamma_k\langle c^\dagger_{k\sigma}c_{k\sigma}\rangle$ into calculations. In Eqs (2), (4), (8) – (10), ε_k must be changed into $\tilde{\varepsilon}_k = \varepsilon_k(1 + pW/zt)$ then, and we have to solve Eqs (8) – (10) self consistently with the equation for the Fock term: $p = -\frac{1}{N}\sum_k \tilde{\varepsilon}_k\gamma_k F_k$. Equations (11) – (12) remain valid, with the change $X \to X/(1 + pW/zt)$ where $X = \mu$, W_{cr} and U.

III. LOW DENSITY LIMIT

Going back to Hamiltonian Eq. (1) we can obtain exact results in the low density limit. In the center-of-mass coordinate system we can expand the wave function of the two-electron bound pair ψ in the basis of plane

waves (i.e., eigenstates of the hopping part of the Hamiltonian Eq. (1)). We can easily find the equations for the coefficients of the expansion, what finally yields a set of self-consistent equations for the wave function in the position space, in terms of lattice Green functions [2, 17]:

$$\psi(\mathbf{r}) = \sum_{\mathbf{r}'} G(E, \mathbf{P}, \mathbf{r}, \mathbf{r}') g(\mathbf{r}') \psi(\mathbf{r}') \ , \tag{13}$$

where G is lattice Green function defined by:

$$G(E, \mathbf{P}, \mathbf{r}, \mathbf{r}') = \frac{1}{N} \sum_{q} \frac{e^{i\mathbf{q}\cdot\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}'}}{E - E_{\mathbf{Pq}}} \ , \tag{14}$$

and $g(\mathbf{r})$ is diagonal interaction matrix, consisting of elements U and W. Eigenenergy equation takes the form:

$$det[\mathcal{G} - g^{-1}] = 0 \ , \tag{15}$$

where $\mathcal{G}$ is a matrix with elements $\mathcal{G}_{ij} = G(E, \mathbf{P}, \mathbf{r}_i, \mathbf{r}_j)$. This is an analogue of Eqs (8) – (9). Let's note that in the case of the two-electron bound pairs $\Delta = 0$ and the role of the binding energy is played by $\overline{\mu}/2$. For the hypercubic lattices these equations were solved and it has been found out that in one and two dimensions pairs for $W = 0$ bind for any negative U, while in three dimensions there is critical value for W [18]. The formula for W_{cr} in the case of two-electron bound state reads [2]:

$$\frac{|W_{cr}|}{2t} = \left[1 + \frac{2D}{U}\right]^{-1} + (\overline{C} - 1)^{-1} \ , \tag{16}$$

where $\overline{C} = 1/N \sum_k (1 - \gamma_k/z)^{-1}$ is the Watson integral. This is an exact result. Remembering that $\overline{C}$ is divergent for lattices of dimensions $d = 1$ and $d = 2$ we can see, that for $n \to 0$ $\mu/D \to -1$, $I \to 0$ (Eq. (11)) and Eq. (16) is a limiting value of the formula Eqs (11) and (12) for $d = 1$ and $d = 2$, as it should be. Not for $d = 3$ though; this case will be discussed later on.

Let's note that Eqs (11), (12) and (16), are valid for any combination of signs of U and W and for large enough $U < 0$ and $W < 0$ there is a second branch of solutions [16, 19]. The two branches are the two solutions which realize in the two opposite limits: $U = +\infty$ and $U = -\infty$ (or $W = \pm\infty$). The formal equations and their solutions in both these limits are the same, despite completely different physical situation. Nevertheless these are the specific cases of two distinct solutions.

IV. RESULTS AND DISCUSSION

In view of the Randeria's notice, described in the Introduction, in the case of s-wave symmetry in two dimensions we can use condition for existence of bound states as a condition for existence of superconductivity. In Fig. 1 the boundaries expressed by Eq. (11) for different lattice dimensionalities and electron densities are shown. For parameters U, W belonging to the area above the plotted lines (mostly in the 1st quarter of coordinate system) two-electron bound states, and what follows s-wave superconductivity in two dimensions, can not exist. The curves for $n = 0$ in all dimensions are exact results.

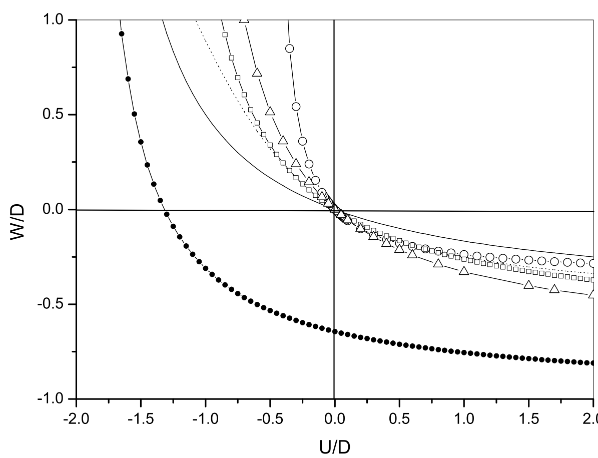

FIG. 1: Critical values for existence of bound pairs and superconductivity for: $n = 0$ for $d = 3$ (black circles - bound pairs only), $n = 0$ and rectangular DOS (full line), $n = 0.25$, rectangular DOS and Fock term (dotted line), $n = 0.25$ and rectangular DOS (squares), $n = 0.25$ for $d = 2$ (triangles) and $n = 0.25$ for $d = 3$ (white circles - superconductivity only). Line $n = 0$ for $d = 2$ is the same as for the rectangular DOS. Half-bandwidth unit $D = 4t$ for rectangular DOS and for $d = 2$ while $D = 6t$ for $d = 3$.

As n gets larger, the area of existence of bound pairs increases for $W > 0$ and $U < 0$ and decreases in the part of the diagram with $W < 0$ and $U > 0$. All curves except the one for $n = 0$ in $d = 3$ go through the point

with coordinates $(0,0)$. This illustrates the fact that for $W = 0$ infinitesimally small U creates bound state in $d = 2$, while the threshold exists in $d = 3$. Nevertheless we do not have threshold in $d = 3$ for $n \neq 0$ – in agreement with Randeria's notion about necessity of bound states for superconductivity only in $d = 2$. Let's note that for large U and W the curves approach the asymptotes – for curves crossing through the axes origin the asymptotes are given by the formulas: $U_{as}/t = -16(n-1)^2/(1+(n-1)^2)$ and $W_{as}/t = -4/(1+(n-1)^2)$. This is connected with the fact that in the 3rd quarter of the coordination system for $U < 0$ and $W < 0$ there exist second branches of the solutions. As they have higher energy than the solutions described in Fig. 1 they do not modify the ground state phase diagram and are not shown here.

The dotted line in Fig. 1 (and in Fig. 2) describes the results of calculations with inclusion of the Fock term, using Eq. (12) modified by the $(1 + pW/zt)$ term, as was described in the end of Section 2. To simplify the calculations the Fock term from the normal state was used: $p = n(2-n)$. For $W > 0$ this term broadens the band moving the system more into weak coupling limit and enlarging the normal state area (opposite behavior for $W < 0$). The same effect can be seen in Fig. 2.

In Fig. 2 the boundaries of existence of bound states, Eq. (12) (black symbols), are plotted on a ground state phase diagram of the extended Hubbard model for $U < 0$ and $W > 0$, for arbitrary n and rectangular DOS, together with the phase boundary PS[CDW/SS]/SS taken from Ref. [12] (white symbols). Above the lines with black symbols s-wave superconductivity can not exist in $d = 2$. This way the superconducting state is suppressed and normal state (NO) area is introduced into the phase diagram. Let's note that also the phase separated state PS[CDW/SS] is "reduced" to the NO phase and not to the CDW phase. This is due to the fact that the CDW in the PS state is the CDW with $n = 1$. CDW with $n \neq 1$ is unstable, as it has negative compressibility.

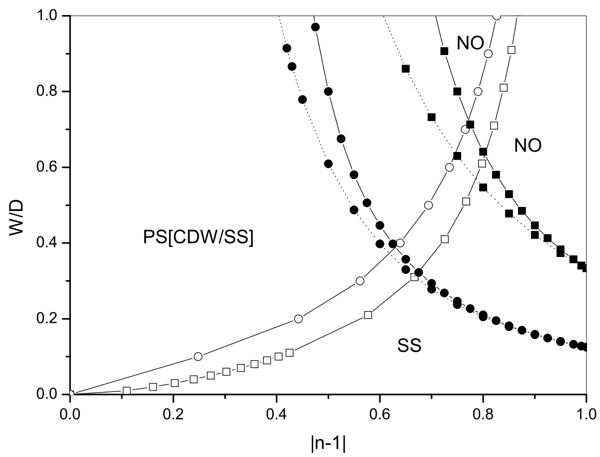

FIG. 2: Phase boundaries for $U/D = -0.4$ (circles) and $U/D = -0.8$ (squares) calculated for the rectangular DOS. Black symbols denote boundary of existence of bound state, white symbols boundary between singlet superconductivity (SS) and phase separated area PS[CDW/SS] (with charge density wave CDW and SS). Symbols on dotted lines show the results of calculations including Fock term.

Another thing to note is the threshold for appearance of bound states for $n = 0$, which increases with increasing $|U|$. The phase diagram is modified only for intermediate values of $|U|$ and $|W|$, smaller from their asymptotic values $|U_{as}|$ and $|W_{as}|$. For $|U|$ or $|W|$ larger than these values, bound states exist for arbitrary value of the other parameter, in agreement with Fig. 1.

The calculations in Ref. [12] consider only pure, on-site s-wave pairing. Including Δ_γ (Eq. (9)) into calculations does not change much the described PS[CDW/SS]/SS boundary – Δ_γ is two orders of magnitude smaller than Δ_0 on this boundary. Inclusion of Fock term into the calculations of the bound states, results in extending the area of the normal phase, as was mentioned before. This effect increases with increasing $|n|$ and W.

In conclusion it was shown, how the analytical (and exact for $n = 0$) formulas for bound two-electron states can be used for the modification of the $U < 0$, $W > 0$ part of the phase diagram of the extended Hubbard model. The main result of this approach is suppression of the superconducting and phase separated areas in favor of the normal phase around half-filled band for intermediate values of $|U|$ and $|W|$, larger than threshold values and smaller than $|U_{as}|$ and $|W_{as}|$.

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